wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 11:37 AM EST

PDB ID	:	1FBX
Title	:	CRYSTAL STRUCTURE OF ZINC-CONTAINING E.COLI GTP CYCLO-HYDROLASE I
Authors	:	Auerbach, G.; Herrmann, A.; Bracher, A.; Bader, A.; Gutlich, M.; Fischer, M.; Neukamm, M.; Nar, H.; Garrido-Franco, M.; Richardson, J.; Huber, R.; Bacher, A.
Deposited on	:	2000-07-17
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

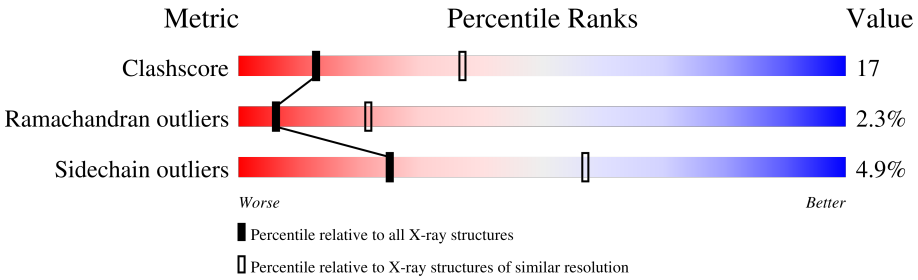
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	69% 29% ·
1	B	221	72% 25% ·
1	C	221	76% 23% ·
1	D	221	73% 24% ·
1	E	221	65% 33% ·
1	F	221	68% 29% ·
1	G	221	70% 29% ·
1	H	221	69% 28% ·

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Mol	Chain	Length	Quality of chain
1	I	221	60% 36%
1	J	221	65% 32%
1	K	221	67% 30%
1	L	221	63% 33%
1	M	221	64% 33%
1	N	221	58% 39%
1	O	221	62% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	3350	-	-	X	-
3	CL	F	3355	-	-	X	-
3	CL	J	3354	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26025 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	B	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	C	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	D	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	E	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	F	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	G	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	H	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	I	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	J	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	K	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	L	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	M	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	N	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			
1	O	221	Total	C	N	O	S	74	0	0
			1732	1088	309	326	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0
2	N	1	Total Zn 1 1	0	0
2	O	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0
3	N	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0
4	L	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	1	Total O 1 1	0	0
4	O	1	Total O 1 1	0	0

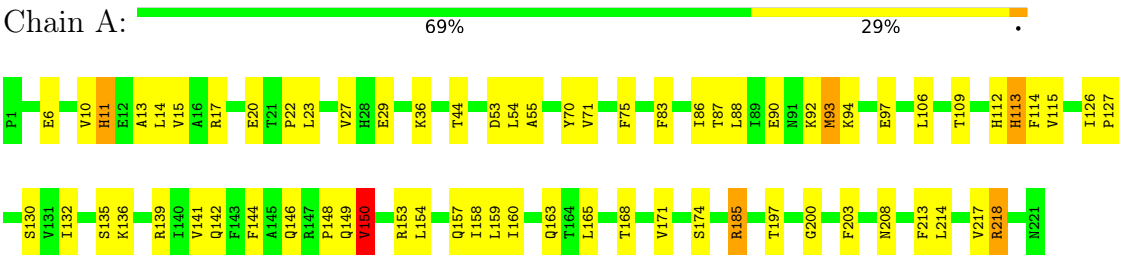
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

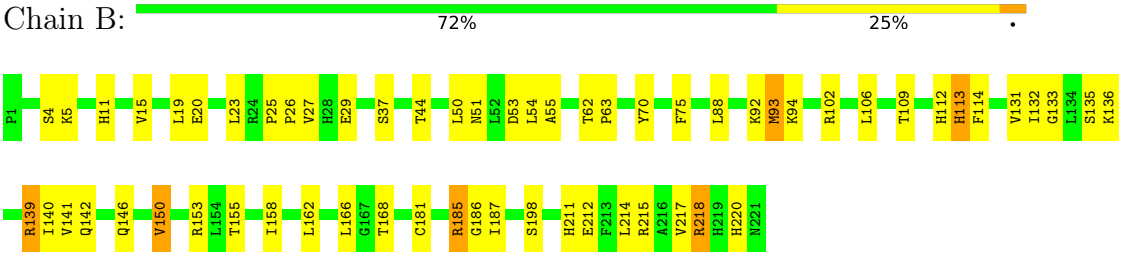
• Molecule 1: GTP CYCLOHYDROLASE I

Chain A:



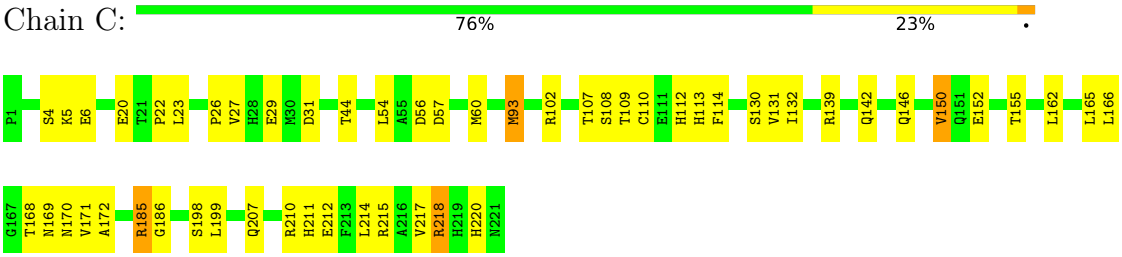
• Molecule 1: GTP CYCLOHYDROLASE I

Chain B:



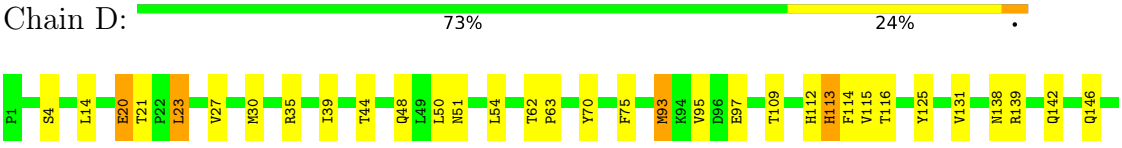
• Molecule 1: GTP CYCLOHYDROLASE I

Chain C:



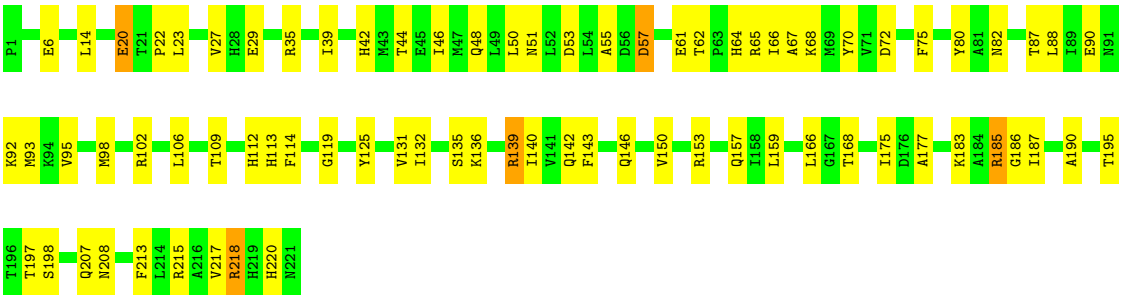
• Molecule 1: GTP CYCLOHYDROLASE I

Chain D:



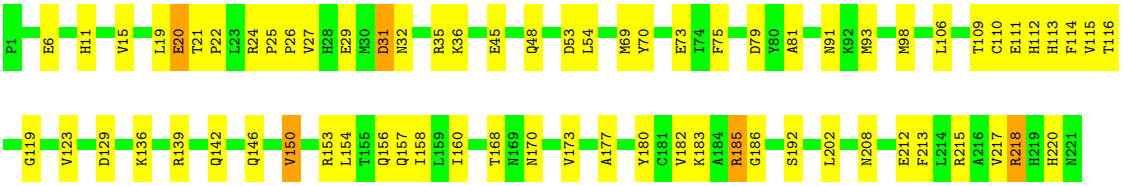
• Molecule 1: GTP CYCLOHYDROLASE I

Chain E:



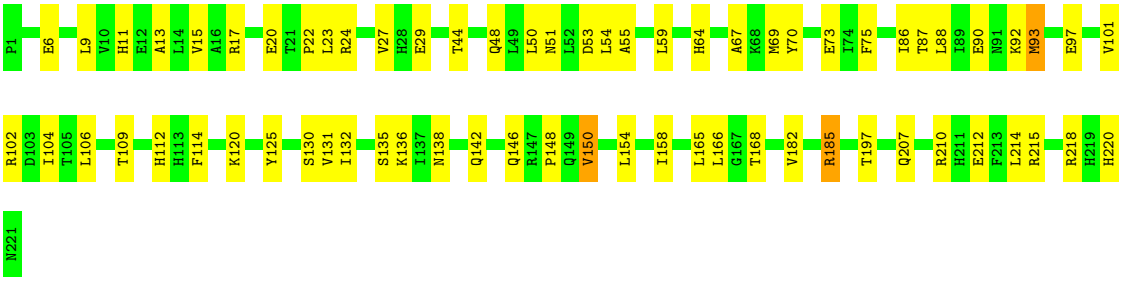
• Molecule 1: GTP CYCLOHYDROLASE I

Chain F:



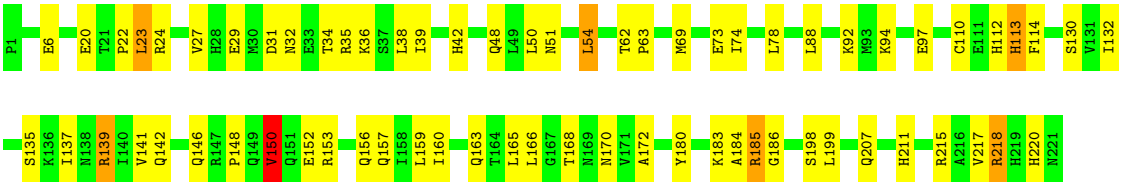
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G:



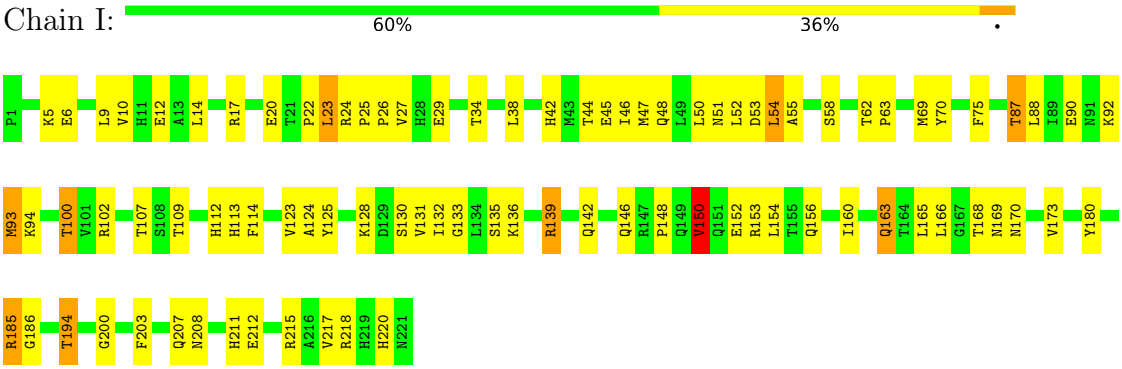
• Molecule 1: GTP CYCLOHYDROLASE I

Chain H:



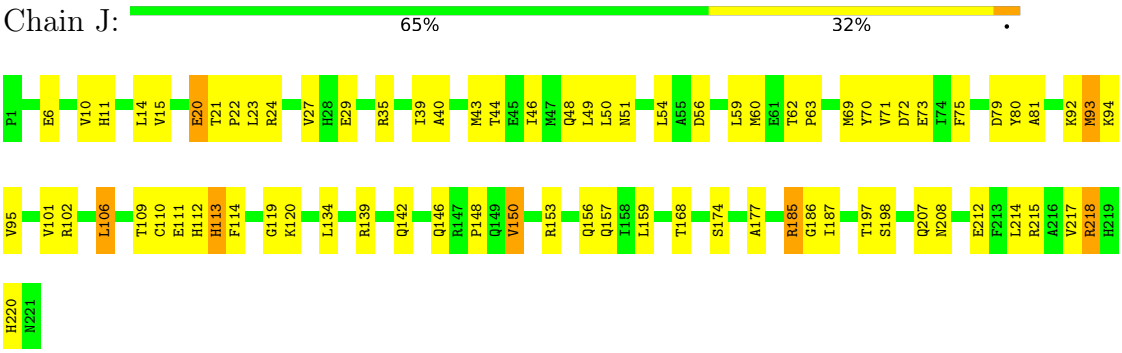
• Molecule 1: GTP CYCLOHYDROLASE I

Chain I:



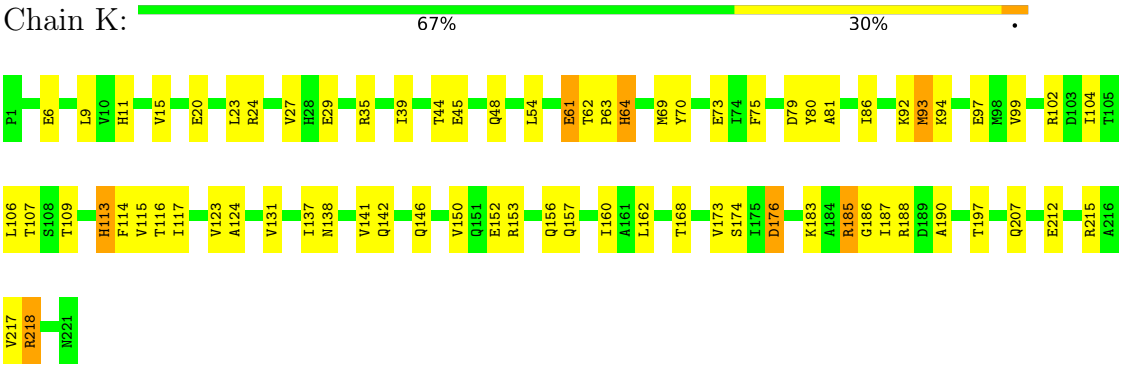
• Molecule 1: GTP CYCLOHYDROLASE I

Chain J:



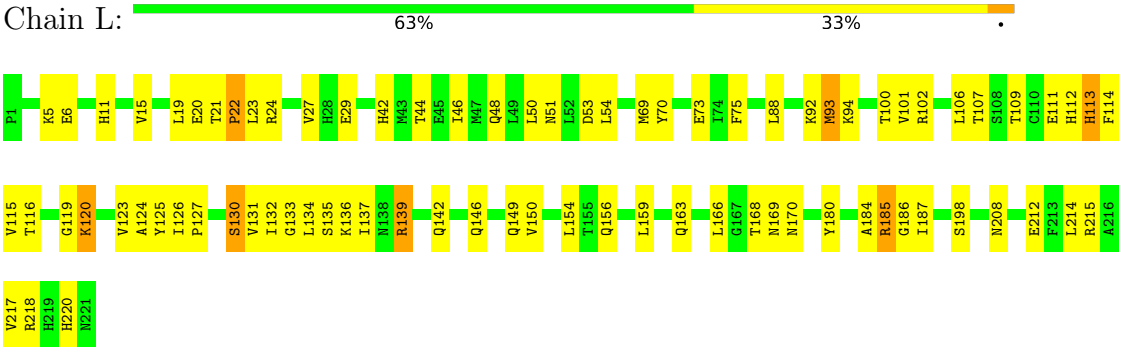
• Molecule 1: GTP CYCLOHYDROLASE I

Chain K:



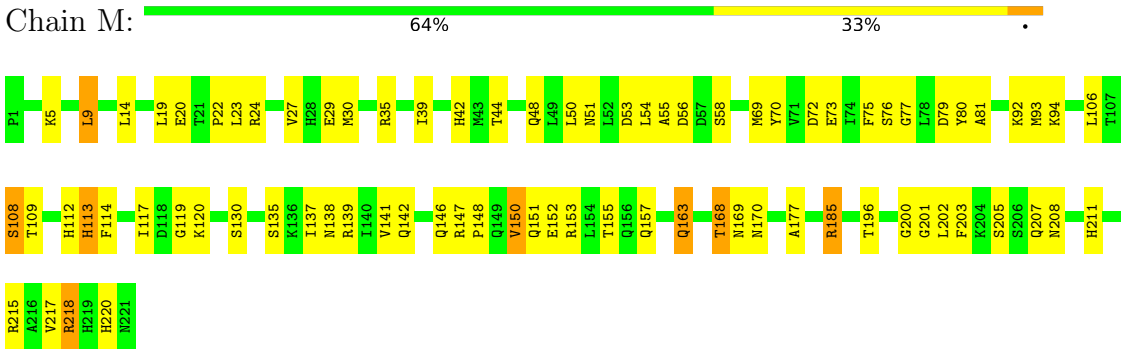
• Molecule 1: GTP CYCLOHYDROLASE I

Chain L:



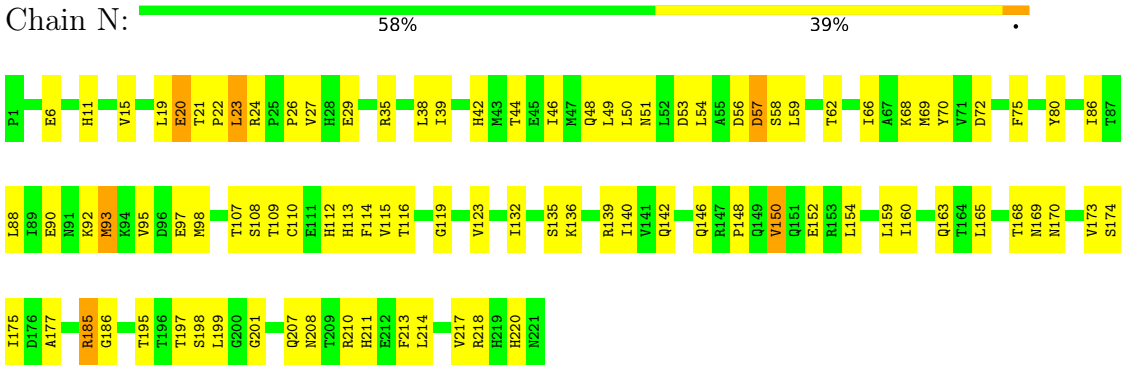
• Molecule 1: GTP CYCLOHYDROLASE I

Chain M:



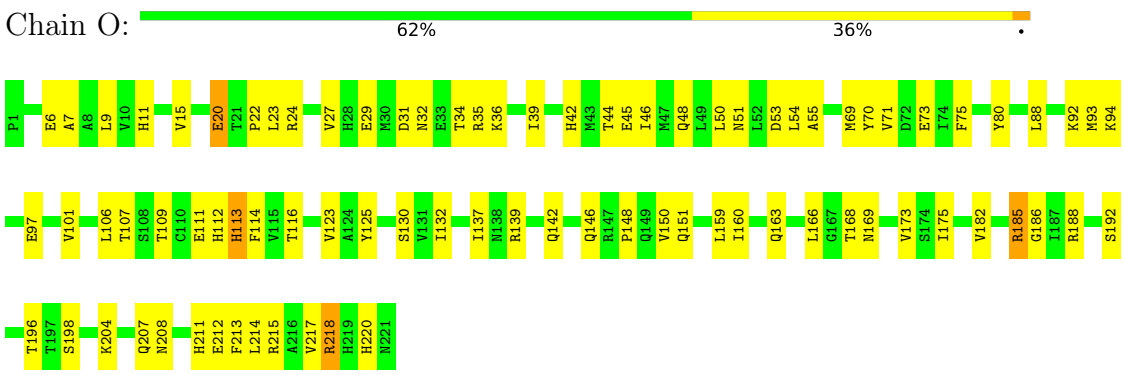
• Molecule 1: GTP CYCLOHYDROLASE I

Chain N:



• Molecule 1: GTP CYCLOHYDROLASE I

Chain O:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	227.69Å 314.19Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.80	Depositor
% Data completeness (in resolution range)	91.2 (14.98-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26025	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	0/1760	0.80	1/2384 (0.0%)
1	B	0.59	1/1760 (0.1%)	0.81	1/2384 (0.0%)
1	C	0.60	0/1760	0.84	1/2384 (0.0%)
1	D	0.58	0/1760	0.80	0/2384
1	E	0.50	0/1760	0.78	0/2384
1	F	0.52	0/1760	0.77	1/2384 (0.0%)
1	G	0.45	0/1760	0.72	1/2384 (0.0%)
1	H	0.52	0/1760	0.77	2/2384 (0.1%)
1	I	0.47	0/1760	0.73	1/2384 (0.0%)
1	J	0.51	0/1760	0.77	1/2384 (0.0%)
1	K	0.54	2/1760 (0.1%)	0.76	1/2384 (0.0%)
1	L	0.45	0/1760	0.71	0/2384
1	M	0.52	0/1760	0.77	1/2384 (0.0%)
1	N	0.47	0/1760	0.72	0/2384
1	O	0.47	0/1760	0.72	0/2384
All	All	0.52	3/26400 (0.0%)	0.77	11/35760 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	61	GLU	CG-CD	6.46	1.61	1.51
1	B	181	CYS	CB-SG	-5.54	1.72	1.81
1	K	61	GLU	CB-CG	5.46	1.62	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	150	VAL	N-CA-C	-6.06	94.63	111.00
1	H	150	VAL	N-CA-C	-6.00	94.80	111.00
1	K	150	VAL	N-CA-C	-5.98	94.86	111.00
1	J	150	VAL	N-CA-C	-5.82	95.29	111.00
1	I	150	VAL	N-CA-C	-5.68	95.67	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	180	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	0	1766	50	0
1	B	1732	0	1766	44	0
1	C	1732	0	1766	39	0
1	D	1732	0	1766	38	0
1	E	1732	0	1766	52	0
1	F	1732	0	1766	68	0
1	G	1732	0	1766	66	0
1	H	1732	0	1766	63	0
1	I	1732	0	1766	86	0
1	J	1732	0	1766	86	0
1	K	1732	0	1766	69	0
1	L	1732	0	1766	73	0
1	M	1732	0	1766	80	0
1	N	1732	0	1766	92	0
1	O	1732	0	1766	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	2	0
3	G	1	0	0	1	0
3	H	1	0	0	1	0
3	I	1	0	0	1	0
3	J	1	0	0	2	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	1	0
3	O	1	0	0	1	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	2	0
4	G	1	0	0	1	0
4	H	1	0	0	2	0
4	I	1	0	0	1	0
4	J	1	0	0	3	0
4	K	1	0	0	0	0
4	L	1	0	0	1	0
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	2	0
All	All	26025	0	26490	835	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 835 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:MET:HE2	1:N:185:ARG:HD2	1.31	1.11
1:C:168:THR:HG22	1:C:170:ASN:H	1.14	1.11
1:I:168:THR:HG22	1:I:170:ASN:H	1.22	1.04
1:F:185:ARG:HD2	1:M:69:MET:HE2	1.38	1.03
1:K:61:GLU:OE1	1:K:64:HIS:HD2	1.41	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/221 (99%)	206 (94%)	9 (4%)	4 (2%)	8	28
1	B	219/221 (99%)	204 (93%)	11 (5%)	4 (2%)	8	28
1	C	219/221 (99%)	200 (91%)	13 (6%)	6 (3%)	5	17
1	D	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	11	34
1	E	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	5	17
1	F	219/221 (99%)	196 (90%)	17 (8%)	6 (3%)	5	17
1	G	219/221 (99%)	195 (89%)	20 (9%)	4 (2%)	8	28
1	H	219/221 (99%)	202 (92%)	11 (5%)	6 (3%)	5	17
1	I	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	5	17
1	J	219/221 (99%)	196 (90%)	18 (8%)	5 (2%)	6	21
1	K	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	8	28
1	L	219/221 (99%)	191 (87%)	24 (11%)	4 (2%)	8	28
1	M	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	5	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	219/221 (99%)	196 (90%)	16 (7%)	7 (3%)	4 13
1	O	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	5 17
All	All	3285/3315 (99%)	2979 (91%)	229 (7%)	77 (2%)	6 21

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	218	ARG
1	B	27	VAL
1	F	27	VAL
1	K	27	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/194 (100%)	185 (95%)	9 (5%)	27 60
1	B	194/194 (100%)	186 (96%)	8 (4%)	30 64
1	C	194/194 (100%)	183 (94%)	11 (6%)	20 50
1	D	194/194 (100%)	183 (94%)	11 (6%)	20 50
1	E	194/194 (100%)	182 (94%)	12 (6%)	18 47
1	F	194/194 (100%)	190 (98%)	4 (2%)	53 84
1	G	194/194 (100%)	184 (95%)	10 (5%)	23 55
1	H	194/194 (100%)	186 (96%)	8 (4%)	30 64
1	I	194/194 (100%)	180 (93%)	14 (7%)	14 38
1	J	194/194 (100%)	185 (95%)	9 (5%)	27 60
1	K	194/194 (100%)	185 (95%)	9 (5%)	27 60
1	L	194/194 (100%)	187 (96%)	7 (4%)	35 69
1	M	194/194 (100%)	180 (93%)	14 (7%)	14 38
1	N	194/194 (100%)	184 (95%)	10 (5%)	23 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	194/194 (100%)	186 (96%)	8 (4%)	30 64
All	All	2910/2910 (100%)	2766 (95%)	144 (5%)	25 57

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	30	MET
1	O	185	ARG
1	M	120	LYS
1	N	107	THR
1	E	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	163	GLN
1	O	113	HIS
1	J	112	HIS
1	O	112	HIS
1	N	48	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.